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|--|-------|--------|---|
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| NEWS   | 2     | JAN 02 | STN pricing information for 2008 now available  |
| NEWS   | 3     | JAN 16 | CAS patent coverage enhanced to include exemplified prophetic substances              |
| NEWS   | 4     | JAN 28 | USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats          |
| NEWS   | 5     | JAN 28 | MARPAT searching enhanced   |
| NEWS   | 6     | JAN 28 | USGENE now provides USPTO sequence data within 3 days of publication                  |
| NEWS   | 7     | JAN 28 | TOXCENTER enhanced with reloaded MEDLINE segment                                      |
| NEWS   | 8     | JAN 28 | MEDLINE and LMEDLINE reloaded with enhancements                                       |
| NEWS   | 9     | FEB 08 | STN Express, Version 8.3, now available   |
| NEWS   | 10    | FEB 20 | PCI now available as a replacement to DPCI  |
| NEWS   | 11    | FEB 25 | IFIREF reloaded with enhancements   |
| NEWS   | 12    | FEB 25 | IMSPRODUCT reloaded with enhancements   |
| NEWS   | 13    | FEB 29 | WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification |
| NEWS   | 14    | MAR 31 | IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats               |
| NEWS   | 15    | MAR 31 | CAS REGISTRY enhanced with additional experimental spectra                            |
| NEWS   | 16    | MAR 31 | CA/CAPplus and CASREACT patent number format for U.S. applications updated            |
| NEWS   | 17    | MAR 31 | LPCI now available as a replacement to LDPCI  |
| NEWS   | 18    | MAR 31 | EMBASE, EMBAL, and LEMBASE reloaded with enhancements                                 |
| NEWS   | 19    | APR 04 | STN AnaVist, Version 1, to be discontinued  |
| NEWS   | 20    | APR 15 | WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats             |
| NEWS   | 21    | APR 28 | EMBASE Controlled Term thesaurus enhanced   |
| NEWS   | 22    | APR 28 | IMSRESEARCH reloaded with enhancements  |
| NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,<br>AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008 |       |        |   |
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| NEWS   | IPC8  |        | For general information regarding STN implementation of IPC 8                         |

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 06:40:29 ON 20 MAY 2008

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 06:40:38 ON 20 MAY 2008

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STRUCTURE FILE UPDATES: 19 MAY 2008 HIGHEST RN 1021481-05-9

DICTIONARY FILE UPDATES: 19 MAY 2008 HIGHEST RN 1021481-05-9

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

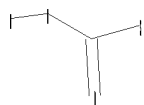
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10591283.str



chain nodes :

1 2 3 4 5

chain bonds :

1-2 1-3 3-4 3-5

exact/norm bonds :

1-3 3-4 3-5

exact bonds :

1-2

Match level :

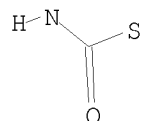
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 06:41:43 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1777 TO ITERATE

100.0% PROCESSED 1777 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 33012 TO 38068

PROJECTED ANSWERS: 8435 TO 11085

L2 50 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 06:41:51 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 35791 TO ITERATE

100.0% PROCESSED 35791 ITERATIONS

9686 ANSWERS

SEARCH TIME: 00.00.01

L3 9686 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

178.82

179.03

FILE 'CAPLUS' ENTERED AT 06:41:58 ON 20 MAY 2008

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FILE COVERS 1907 - 20 May 2008 VOL 148 ISS 21

FILE LAST UPDATED: 19 May 2008 (20080519/ED)

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<http://www.cas.org/legal/infopolicy.html>

=> s 13

L4 5006 L3

=> s 14 and thiocarbamide

1137 THIOCARBAMIDE

L5 12 L4 AND THIOCARBAMIDE

=> DIS L5 1 IBIB IABS

L5 ANSWER 1 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:371036 CAPLUS

DOCUMENT NUMBER: 140:377715

TITLE: Method for producing lubricant additive (variants)

INVENTOR(S): Bakunin, Viktor Nikolaevich; Kuz'mina, Galina

Nikolaevna; Parenago, Oleg Pavlovich

PATENT ASSIGNEE(S): Institut Neftekhimicheskogo Sinteza Ran Im. A. V.

Topchieva (Inkhs Ran), Russia

SOURCE: PCT Int. Appl., 19 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Russian

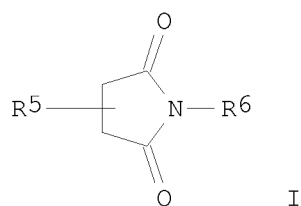
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO.  | DATE       |
|---|------|----------|------------------|------------|
| WO 2004037957   | A1   | 20040506 | WO 2003-RU440    | 20031016   |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW |      |          |                  |            |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG                        |      |          |                  |            |
| AU 2003277760   | A1   | 20040513 | AU 2003-277760   | 20031016   |
| GB 2411660  | A    | 20050907 | GB 2005-10381    | 20031016   |
| GB 2411660  | B    | 20060712 |                  |            |
| DE 10393575   | T5   | 20050929 | DE 2003-10393575 | 20031016   |
| CN 1723269  | A    | 20060118 | CN 2003-80105316 | 20031016   |
| JP 2006503954   | T    | 20060202 | JP 2004-546580   | 20031016   |
| US 20060094605  | A1   | 20060504 | US 2005-532416   | 20050906   |
| PRIORITY APPLN. INFO.:  |      |          | RU 2002-128364   | A 20021023 |
|   |      |          | WO 2003-RU440    | W 20031016 |

OTHER SOURCE(S): MARPAT 140:377715

GRAPHIC IMAGE:



ABSTRACT:

The invention relates to petroleum chemical, and more specifically to sulfur-containing molybdenum compds. and to the use thereof as lubricant additives which decrease friction coefficient. In the 1st variant, molybdenum trisulfide nanoparticles and the derivs. thereof are produced from thio-molybdenum acid salts  $M_2MoS_4-xO_x$ , wherein  $M = NH_4, Na$ ,  $x = 0-3$  in the presence of two modifiers, one of them being embodied as tetra-alkyl-ammonium salts or a mixture of salt  $R_1R_2R_3R_4NX$ , wherein  $R_1R_2R_3$  and  $R_4$  equal or different are selected from a group containing  $C_1-C_{16}$  alkyl,  $X = Cl, Br$ , the 2nd modifier being embodied as a succinimide Formula I, wherein  $R_5$  = straight or branched-chain alkyl or oligoalkylene whose molar mass ranges from 140 to .apprx.1000,  $R_6$  is selected from a group comprising  $H, -C(=O)NH_2, -(CH_2CH_2NH)nMe$ ,  $n = 1-4$ . The process is carried out by a thermal treatment and the additive is homogenized in the polar solvent of the mixture of a thio-molybdenum acid salt and the 1st or 2nd modifier, cooling the thus produced mixture and a subsequently adding the 2nd or the 1st modifier, resp. In the 2nd variant, the inventive method consists in producing molybdenum trisulfide nanoparticles and the derivs. thereof from molybdenum acid salts  $M_2MoO_4$ , wherein  $M = NH_4, Na$ , and a sulfur donator embodied as an inorg. sulfide or a polysulfide  $M'_2Sn$ , wherein  $M' = M = NH_4, Na$ ,  $n = 1-4$ , or a thiocarbamide, afterwards, the 1st variant being used.

=> DIS L5 2 IBIB IABS

L5 ANSWER 2 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:808727 CAPLUS

DOCUMENT NUMBER: 134:103528

TITLE: Solvent-free reactive extraction. Metal recovery from leaching solutions, process baths and wastewater using N-acylthiocarbamic acid ester

AUTHOR(S): Heil, Gunter

CORPORATE SOURCE: FH Aachen, FB Chemieingenieurwesen, Germany

SOURCE: Umwelt (2000), 30(9), 48-53

CODEN: UMWLDA; ISSN: 0041-6355

PUBLISHER: Springer-VDI-Verlag GmbH & Co. KG

DOCUMENT TYPE: Journal

LANGUAGE: German

ABSTRACT:

A new procedure for the solvent-free reactive extraction of Cu, Ag, Au, or platinum-metals from watery solns. is described. N-benzoylthiocarbamic acid-o-alkyl ester and N-acylthiocarbamic acid ester, dissolved in ethanol or alkaline solution, were used as complexing agents. Extraction yields of  $Cu^{2+}$ ,  $Ni^{3+}$ , and  $Zn^{2+}$  were determined in dependence on pH. The advantages and disadvantages of both, the new and the classical method are compared.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> DIS L5 3 IBIB IABS

L5 ANSWER 3 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:124488 CAPLUS

DOCUMENT NUMBER: 128:194984

TITLE: Characteristics of depressing action of low-molecular organic compounds in selection of copper-molybdenum concentrates

AUTHOR(S): Desyatov, A. M.; Khersonskii, M. I.; Kondrat'eva, L. V.; Maiorov, A. D.

CORPORATE SOURCE: GNTs RF "Gintsvetmet", Russia

SOURCE: Obogashchenie Rud (Sankt-Peterburg) (1997), (5), 12-16

CODEN: OBOGAD; ISSN: 0202-3776

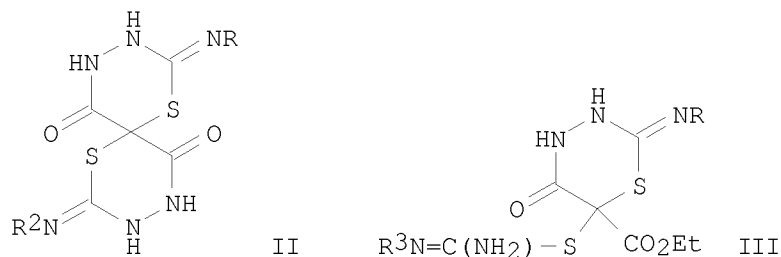
PUBLISHER: Institut Mekhanobr  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
ABSTRACT:

Various flotation agents selected from thiocarbamic acid derivs. acting as depressors of Cu in flotation of Co-Mo ores were developed to decrease the reagent and energy consumption. Synthesis and the mechanism of depression action of the flotation agents are considered.

=> DIS L5 4 IBIB IABS

L5 ANSWER 4 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:653591 CAPLUS  
DOCUMENT NUMBER: 123:256652  
ORIGINAL REFERENCE NO.: 123:45903a, 45906a  
TITLE: A new approach to the chemistry of spiroheterocycles  
AUTHOR(S): Chande, Madhukar S.; Paingankar, Niranjan M.  
CORPORATE SOURCE: Dep. Chem., Inst. Sci., Bombay, 400 032, India  
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1995), 34B(7), 603-6  
CODEN: IJSBDB; ISSN: 0376-4699  
PUBLISHER: Publications & Information Directorate, CSIR  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 123:256652  
GRAPHIC IMAGE:



ABSTRACT:

Interaction of di-Et  $\alpha,\alpha$ -dibromomalonate (I) with 4-substituted thiosemicarbazides in the presence of a base afford spiro compds. II [R, R<sub>2</sub> = H, (un)substituted Ph]. However, in the absence of base, di-Et bis[N-aminocarbamylmercapto]malonate [H<sub>2</sub>NNHC(O)S]<sub>2</sub>C(CO<sub>2</sub>Et)<sub>2</sub> is obtained exclusively. Similarly, the reactions of I with 1-phenyl-4-substituted thiosemicarbazides are reported. Interaction of I with thiosemicarbazides in the presence of thiocarbamides R<sup>3</sup>NHC(S)NH<sub>2</sub> [R<sup>3</sup> = H, (un)substituted Ph] afford 1,3,4-thiadiazin-5-ones, e.g. III [R, R<sup>3</sup> = H, (un)substituted Ph].

=> DIS L5 5 IBIB IABS

L5 ANSWER 5 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:319673 CAPLUS

DOCUMENT NUMBER: 122:88128  
ORIGINAL REFERENCE NO.: 122:16567a,16570a  
TITLE: Occupational contact dermatitis induced by allergens present in rubber  
AUTHOR(S): Kiec-Swierczynska, Marta  
CORPORATE SOURCE: Clinic of Occupational Diseases, Jerzy Nofer Inst. of Occupational Medicine, Lodz, Pol.  
SOURCE: Medycyna Pracy (1994), 45(4), 303-9  
CODEN: MEPAAX; ISSN: 0465-5893  
PUBLISHER: Instytut Medycyny Pracy  
DOCUMENT TYPE: Journal  
LANGUAGE: Polish  
ABSTRACT:  
Thiurams, thiocarbamates, thiazoles, guanidine derivs., and \*\*\*thiocarbamide\*\*\* were the most frequent causes of occupational dermatitis developed on contact with rubber.

=> DIS L5 6 IBIB IABS

L5 ANSWER 6 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:250176 CAPLUS  
DOCUMENT NUMBER: 114:250176  
ORIGINAL REFERENCE NO.: 114:42215a,42218a  
TITLE: Separation of isocyanic acid from gaseous ammonia-isocyanic acid mixtures  
INVENTOR(S): Muellner, Martin; Stern, Gerhard; Erich, Schulz  
PATENT ASSIGNEE(S): Chemie Linz G.m.b.H., Austria  
SOURCE: Eur. Pat. Appl., 8 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE        |
|---|------|----------|-----------------|-------------|
| -----   | ---  | -----    | -----           | -----       |
| EP 416236   | A2   | 19910313 | EP 1990-112744  | 19900704    |
| EP 416236   | A3   | 19940727 |                 |             |
| EP 416236   | B1   | 19951108 |                 |             |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE |      |          |                 |             |
| AT 129987   | T    | 19951115 | AT 1990-112744  | 19900704    |
| ES 2078273  | T3   | 19951216 | ES 1990-112744  | 19900704    |
| US 5078980  | A    | 19920107 | US 1990-552694  | 19900712    |
| ZA 9005766  | A    | 19910529 | ZA 1990-5766    | 19900723    |
| CZ 280732   | B6   | 19960417 | CZ 1990-3679    | 19900724    |
| JP 03066654   | A    | 19910322 | JP 1990-196400  | 19900726    |
| AU 9059936  | A    | 19910131 | AU 1990-59936   | 19900727    |
| AU 624259   | B2   | 19920604 |                 |             |
| HU 54631  | A2   | 19910328 | HU 1990-4662    | 19900727    |
| HU 209125   | B    | 19940328 |                 |             |
| RU 2015945  | C1   | 19940715 | RU 1990-4830771 | 19900727    |
| US 5223635  | A    | 19930629 | US 1991-768369  | 19910925    |
| PRIORITY APPLN. INFO.:                                    |      |          | AT 1989-1828    | A 19890728  |
|   |      |          | AT 1989-1829    | A 19890728  |
|   |      |          | US 1990-552694  | A3 19900712 |

OTHER SOURCE(S): MARPAT 114:250176

ABSTRACT:

The process comprises introducing a tertiary amine or an ether into the gas mixture at 250-600°, and introducing the mixture into an inert diluent to condense the resulting adduct of the isocyanic acid with the amine or ether.

The NH<sub>3</sub>-isocyanic acid mixts. are obtained by thermal decomposition of urea, and used in the manufacture of melamine. The adducts are reacted at -20° to the b.p. of the solvent with a primary or secondary amine, alc., thiol. or compound containing 1 or 2 nonconjugated, olefinic double bonds, to give the asym., substituted ureas, the carbamates, thiocarbamates, or substituted isocyanates. Urea was thermally decomposed at 100 g/h, and the decomposition gases were contacted at 320° with NEt<sub>3</sub>(g) flowing at 255 g/h, and introduced into CHCl<sub>3</sub> at -10° to give an isocyanic acid-NEt<sub>3</sub> adduct at 66% yield.

=> DIS L5 7 IBIB IABS

L5 ANSWER 7 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:77791 CAPLUS

DOCUMENT NUMBER: 110:77791

ORIGINAL REFERENCE NO.: 110:12849a,12852a

TITLE: Timber preservation with wood preservatives without chlorophenol compounds

AUTHOR(S): Varfolomeev, U. A.; Chashina, L. M.; Lebedeva, L. K.

CORPORATE SOURCE: Cent. Mech. Sch., Archangelsk, USSR

SOURCE: Holztechnologie (1988), 29(5), 258-62

CODEN: HLZTAW; ISSN: 0018-3881

DOCUMENT TYPE: Journal

LANGUAGE: German

ABSTRACT:

Basic characteristics of various com. chlorophenol-free wood preservatives are given along with results of laboratory evaluation on their protective action. Although the cost of these preservatives is higher than the cost of chlorophenol-containing preservatives, the use of the former ones is recommended due to lower costs related to environmental protection and application safety.

=> DIS L5 8 IBIB IABS

L5 ANSWER 8 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1984:25240 CAPLUS

DOCUMENT NUMBER: 100:25240

ORIGINAL REFERENCE NO.: 100:3947a,3950a

TITLE: Metal degreasing bath with increased efficiency

INVENTOR(S): Reiter, Arpad

PATENT ASSIGNEE(S): VIDEOTON Elektronikai Vallalat, Hung.

SOURCE: Hung. Teljes, 17 pp.

CODEN: HUXXB

DOCUMENT TYPE: Patent

LANGUAGE: Hungarian

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.             | KIND | DATE     | APPLICATION NO. | DATE     |
|------------------------|------|----------|-----------------|----------|
| -----                  | ---- | -----    | -----           | -----    |
| HU 26782               | A2   | 19830928 | HU 1981-2852    | 19811002 |
| PRIORITY APPLN. INFO.: |      |          | HU 1981-2852    | 19811002 |

ABSTRACT:

An aqueous solution for metal degreasing contains 3 + 10<sup>-4</sup>-3 mol/L nonionic acid-resistant surfactant, preferably polyglycol ether and 10<sup>-4</sup>-3 mol/L thiocarbonyl compound stable in aqueous acid solution at pH ≤7, and optionally other conventional additives. The thiocarbonyl compound is thioamide thiocyanate, and thiocarbamate, or their derivs. A degreasing aqueous solution containing HCl 40, HF 7, Na hexametaphosphate 8, activating solution (containing 0.6 g Pd/L) 60,



alkyl polyglycol ether 10, and KCNS 5 g/L was used at 55° for 3 min for artificially oiled steel and Cu (printed circuit board) or for Sn electroplates on them. The surfaces were clean after degreasing, pickling in HCl (for Sn plating), and the Sn electroplates were continuous, as compared to contaminated, corroded, and porous (defective) for the degreasing solution containing

no KCNS. Other components used were thiocarbamide [\*\*\*19045-66-0\*\*\*], diethyl-dithiocarbamate [147-84-2], polyethylene glycol tributylphenyl ether [9046-09-7], thioformamide [115-08-2], citric acid [77-92-9], and alkylamide polyglycol ether.

=> DIS L5 9 IBIB IABS

L5 ANSWER 9 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1969:501793 CAPLUS

DOCUMENT NUMBER: 71:101793

ORIGINAL REFERENCE NO.: 71:18961a,18964a

TITLE: Isomeric changes involving amidino and thioamidino groups. III. Synthesis and transformations of 2-arylimino-6-acetylimino-tetrahydro-6H-1,3-thiazine and related chemistry

AUTHOR(S): Rao, Y. Ramachandra

CORPORATE SOURCE: Nagpur Univ., Nagpur, India

SOURCE: Indian Journal of Chemistry (1969), 7(8), 772-6

CODEN: IJOCAP; ISSN: 0019-5103

DOCUMENT TYPE: Journal

LANGUAGE: English

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

ABSTRACT:

Cyclization of 1-aryl-3-( $\beta$ -cyanoethyl) thiocarbamide (where aryl = phenyl and p-tolyl) to 2-(arylimino)-6-acetyliminotetrahydro-6H-1,3-thiazine(I) and the transformation of the latter under the influence of a base into 2-thioxo-4-(arylimino)hexahydropyrimidine and related H<sub>2</sub>NCSNHCH<sub>2</sub>CH<sub>2</sub>CONHAr has been reported. Structures of the acetylthiazines and the rearranged products have been confirmed by ir spectral data.

=> DIS L5 10 IBIB IABS

L5 ANSWER 10 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1932:14899 CAPLUS

DOCUMENT NUMBER: 26:14899

ORIGINAL REFERENCE NO.: 26:1586d-i,1587a-d

TITLE: Inhibitory effect of substituents in chemical reactions. II. Reactivity of the isothiocyano group in substituted arylthiocarbimides

AUTHOR(S): Browne, Donald W.; Dyson, George M.

SOURCE: Journal of the Chemical Society (1931) 3285-308

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ABSTRACT:

cf. C. A. 21, 1637. A study is reported of the formation of thiourethans from arylthiocarbimides by prolonged boiling with alcs.: RNCS + R'OH  $\rightarrow$  RN:C(SH)OR' .dblharw. RNHCSOR'. By using 100-150 mols. of alc., it is possible to observe the formation of the thiourethans as an almost unimol. reaction, while, in but 1 or 2 cases, no side reactions were observed to interfere with the detns. made upon the main reaction. The quantity of RNCS remaining in the reaction liquid was detd. by reaction with RNH<sub>2</sub> in hot alc.; PhNH<sub>2</sub> could not be

used but (C<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>)<sub>2</sub> reacted rapidly, giving thioureas which were only very slightly sol. in cold alc. (approx. 0.1% at 15°) and could be estd. gravimetrically. The velocities of reaction between 75 RNCS and EtOH have been detd. and results are given for k + 104 and for the proportion converted at various times. The results demonstrate that the nuclear substituents have a profound effect on the reactivity of the NCS group. Whereas halogen atoms and NO<sub>2</sub> groups (and the MeO and EtO groups in the m-position) accelerate the rate of reaction, alkyl or o- or p-alkoxyl groups retard the addn. The effect of more than 1 substituent is approx. the sum of the effects of the substituents acting alone; the m-substituted compd. is always more reactive than the corresponding o- or p-substituted compd. This result is independent of whether the compd. reacts more readily than PhNCS or otherwise. The reactivity varies with the nature of the substituent group, the NO<sub>2</sub> group being most active in acceleration and the iso-Pr group most active in inhibition. The o-group exhibits an anomalous behavior, in that in some cases it exhibits the usual phenomena of steric behavior and in others does not. The following phenylthiocarbimides are described, being prepd. from the amine HCl salt and CSCl<sub>2</sub>; in case the product is an oil it was characterized as the corresponding phenylthiocarbamide, prepd. by heating with EtOH-NH<sub>3</sub>:4-NO<sub>2</sub>, pale yellow, m. 112°; 3-NO<sub>2</sub>, pale yellow, m. 60°; 3-nitro-o-methyl, deep yellow, m. 70°; 4-fluoro-3-nitro, pale yellow, m. 55°; 4-Et, b. 245° (carbamide, m. 138°); 4-isopropyl, b. 252° (carbamide, m. 134°); 3-F, b. 226-7° (carbamide, m. 116°; sym-bis(3-fluorophenyl)thiocarbamide, m. 144°); 4-F, b. 228, m. 12° (sym-bis-(4-fluorophenyl)thiocarbamide, m. 145°); 5-chloro-o-methyl, m. 36°-[α-(5-chloro-o-tolyl)-β-(β-naphthyl) thiocarbamide, m. 163°]; 6-chloro-m-methyl, pale yellow, b. 270° [α-(6-chloro-m-tolyl)-β-(β-naphthyl) thiocarbamide, m. 154°]; 6-chloro-o-methyl, pale yellow, b. 276° [α-(6-chloro-o-tolyl)-β-(β-naphthyl) thiocarbamide, m. 150°]; 5-chloro-m-methyl, m. 34° (α-5-chloro-m-tolyl-β-p-tolylthiocarbamide, m. 156°); 3-chloro-o-methyl, pale yellow, m. 269° (α-3-chloro-o-tolyl-β-p-tolylthiocarbamide, m. 180°); 4-chloro-o-methyl, pale yellow, b. 268° (carbamide, m. 138°); 2-chloro-p-methyl, pale yellow, b. 263° [α-(2-chloro-p-tolyl)-β-(β-naphthyl) thiocarbamide, m. 149°]; 3-chloro-4,6-dimethyl, b. 278° [α-(6-chloro-m-xylyl)-β-(β-naphthyl) thiocarbamide, m. 154°]; 3-chloro-2,4,6-trimethyl, m. 44° [α-chloromesityl-β-(β-naphthyl)thiocarbamide, m. 181°]; 4-chlorom-methyl, b. 272° [α-4-chloro-m-tolyl-β-(β-naphthyl) \*\*\*thiocarbamide\*\*\*, m. 158°]; 2-chloro-m-methyl, b. 264° [α-2-chloro-m-tolyl-β-(β-naphthyl)carbamide, m. 172°]; 3-chloro-p-methyl, b. 258° (α-3-chloro-p-tolyl-β-p-tolylcarbamide, m. 160°); 2-chloro-3,4,6-trimethyl, m. 36° [α-(5-chloro-6-ψ-cumyl)-β-(β-naphthyl) thiocarbamide, m. 161°]; 3-chloro-p-methoxy, m. 89° [α-(β-chloro-p-anisyl)-β-(β-naphthyl) thiocarbamide, m. 174°]; 4-chloro-m-methoxy, m. 51° [α-(4-chloro-m-anisyl)-β-(α-naphthyl)thiocarbamide, m. 155a]; 5-chloro-o-methoxy, m. 61° (carbamide, m. 133°); 5-chloro-m-methoxy, m. 36° (α-5-chloro-m-anisyl-β-p-tolylthiocarbamide, m. 136°); 3,5-dimethoxy, m. 51°-(α-3,5-dimethoxyphenyl-β-p-tolylthiocarbamide, m. 148°); benzaldehyde-4-thiocarbimide, golden, m. 71°; 3-isomer, m. 42°; diphenyl-4-thiocarbimide (xenylthiocarbimide), m. 64°. During the work the following phenylthiourethans were prepd.: 2-NO<sub>2</sub>, lemon-yellow, m. 59°; 3-NO<sub>2</sub>, pale yellow, m. 115°; 4-NO<sub>2</sub>, m. 175°; 2 nitro-3-methyl, pale yellow, m. 110°; 2-nitro-4-methyl, orange-yellow, m. 72°; 2-nitro-6-methyl, pale yellow, m. 109°; 3-nitro-4-methyl, m. 89°; 3-nitro-6-methyl, m. 112°; 4-nitro-2-methyl, m. 116°;

4-nitro-2-methoxy, yellow, m. 76°; 3-nitro-4-fluoro, golden-yellow, m. 118°; 3-Cl, m. 82°; 4-Cl, m. 105°; 2,4-Cl<sub>2</sub>, m. 79°; 2,5-Cl<sub>2</sub>, m. 80°; 3,5-Cl<sub>2</sub>, m. 131°; 3-F, m. 84°; 4-F, m. 86°; 3-Br, m. 94°; 4-Br, m. 107°; 3-I, m. 107°; 4-I, m. 98°; 3-Me, m. 67°; 4-Me, m. 85°; 2,3-Me<sub>2</sub>, m. 108°; 2,5-Me<sub>2</sub>, m. 85°; 3,5-Me<sub>2</sub>, m. 88°; 2-MeO, m. 65°; 3-MeO, m. 85°; 4-MeO, m. 68°; 2,5-(MeO)<sub>2</sub>, m. 72°; 3,4-(MeO)<sub>2</sub>, m. 72°; 3,5-(MeO)<sub>2</sub>, m. 83°; 3-EtO, m. 75°; 4-EtO, m. 95°; 2-chloro-3-methyl, m. 77°; 2-chloro-5-methyl, m. 59°; 3-chloro-2-methyl, m. 88°; 3-chloro-4-methyl, m. 88°; 3-chloro-5-methyl, m. 105°; 3-chloro-6-methyl, m. 81°; 4-chloro-2-methyl, m. 79°; 4-chloro-3-methyl, m. 101°; 3-chloro-4,6-dimethyl, m. 115°; 3-chloro-4-methoxy, m. 96°; 3-chloro-5-methoxy, m. 86°; 3-chloro-6-methoxy, m. 81°; 4-chloro-3-methoxy, m. 124°; 3-CN, m. 95°; 4-CN, m. 110°; 3-aldehydo, m. 147°; 4-aldehydo, m. 135°; 4-Ac, m. 111°; diphenyl-4-thiourethan, m. 117°.

=> DIS L5 11 IBIB IABS

L5 ANSWER 11 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1924:24861 CAPLUS  
 DOCUMENT NUMBER: 18:24861  
 ORIGINAL REFERENCE NO.: 18:3363f-h  
 TITLE: Halogen-substituted aryl thiocarbimides  
 AUTHOR(S): Chattaway, F. D.; Hardy, R. K.; Watts, H. G.  
 SOURCE: Journal of the Chemical Society, Transactions (1924),  
 125, 1552-5  
 CODEN: JCHTA3; ISSN: 0368-1645  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 ABSTRACT:  
 Mixed thiocarbamides can be prepared by the action of PhNCS with halogen-substituted anilines and these decompose to give the halogen-substituted mustard oils when heated with dilute H<sub>2</sub>SO<sub>4</sub>. p-ClC<sub>6</sub>H<sub>4</sub>NCS, m. 44.5°, was obtained in about 30% yield by heating 12.5 g. p-ClC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> and 13.5 g. PhNCS on the H<sub>2</sub>O bath 2-3 hrs., then adding 150 g. H<sub>2</sub>SO<sub>4</sub> diluted with 100 g. H<sub>2</sub>O and distilling with superheated steam. 2,4-Dichlorophenylthiocarbimide, b<sub>17.5</sub> 208°, m. 39°; the corresponding thiocarbamide, m. 158°. Heated with alcs., the alkyl thiocarbamates are formed: Me, m. 48.5°; Et, m. 79°; Pr, m. 72°. 2,4-Dibromophenylthiocarbimide, pale yellow, m. 59.5°; the amide m. 170°; the Et carbamate, m. 62°; Pr ester, m. 68°. Bu phenylthiocarbamate, m. 55°; Bu p-tolylthiocarbamate, m. 65°. p-Chlorophenyl-p-tolylthiocarbamide, m. 173°; p-Br derivative, m. 182°; p-Cl o-tolyl derivative, m. 119.5°. 2,4-Dichlorodiphenylthiocarbamide, m. 157°; 2,4-Br<sub>2</sub> derivative, m. 165°. 2,4-Dichlorophenyl-p-tolylthiocarbamide, m. 145°.

=> DIS L5 12 IBIB IABS

L5 ANSWER 12 OF 12 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1906:75549 CAPLUS  
 DOCUMENT NUMBER: 0:75549  
 TITLE: Monophenylthiocarbamide and imidothiocarbamates  
 AUTHOR(S): Bertram, A.  
 SOURCE: Inaugural Dissertation, Chem. Centr. (1890), (i),  
 939-41

DOCUMENT TYPE: From: J. Chem. Soc., Abstr. 58, 1291-2 1890  
LANGUAGE: Journal  
ABSTRACT: Unavailable

Methyl imidophenylthiocarbamate is obtained by the action of methyl iodide on monophenylthiocarbamide, which forms two sulfates melting at 171°. By means of dry distillation, it is decomposed into aniline, methyl mercaptan, and an unknown compound. When heated with dilute sulfuric acid at 160°, the base yields methyl phenylthiocarbamate. Ethyl iodide combines with monophenylthiocarbamide to form the compounds corresponding with those which it forms with methyl iodide. Ethyl iodide combines with ethyl imidophenylthiocarbamate to yield ethyl imidoethylphenylthiocarbamate, which forms ethyl ethylimidoethylphenylthiocarbamate when heated with ethyl iodide.

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| SINCE FILE | TOTAL   |
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| ENTRY      | SESSION |
| -9.60      | -9.60   |

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L3 9686 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 06:41:58 ON 20 MAY 2008

L4 5006 S L3

L5 12 S L4 AND THIOCARBAMIDE

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SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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ENTRY

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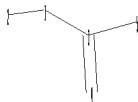
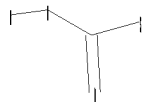
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L6 SCREEN CREATED

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chain nodes :

1 2 3 4 5

chain bonds :

1-2 1-3 3-4 3-5

exact/norm bonds :

1-3 3-4 3-5

exact bonds :

1-2

Match level :  
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS

L7 STRUCTURE UPLOADED

=> que L7 AND L6

L8 QUE L7 AND L6

=> s l8 sss sam  
SAMPLE SEARCH INITIATED 07:09:30 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 504 TO ITERATE

100.0% PROCESSED 504 ITERATIONS 50 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 8734 TO 11426  
PROJECTED ANSWERS: 2477 TO 4003

L9 50 SEA SSS SAM L7 AND L6

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FULL SEARCH INITIATED 07:09:38 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 9904 TO ITERATE

100.0% PROCESSED 9904 ITERATIONS 3337 ANSWERS  
SEARCH TIME: 00.00.01

L10 3337 SEA SSS FUL L7 AND L6

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|  | ENTRY      | SESSION |
| FULL ESTIMATED COST                        | 178.36     | 398.75  |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL   |
|  | ENTRY      | SESSION |
| CA SUBSCRIBER PRICE                        | 0.00       | -9.60   |

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=> s l10 and (carbodiimide OR "Carbodiimides")

1759 L10

12838 CARBODIIMIDE

2865 "CARBODIIMIDES"

L11 7 L10 AND (CARBODIIMIDE OR "CARBODIIMIDES")

=> DIS L11 1 IBIB IABS

L11 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:358147 CAPLUS

Correction of: 2005:481369

DOCUMENT NUMBER: 145:123919

Correction of: 143:26019

TITLE: Carbon dioxide, carbonyl sulfide, carbon disulfide, isocyanates, isothiocyanates, carbodiimides, and their selenium, tellurium, and phosphorus analogues

AUTHOR(S): Braverman, S.; Cherkinsky, M.; Birsa, M. L.

CORPORATE SOURCE: Dept. of Chemistry, Bar-Ilan University, Ramat-Gan, 52900, Israel

SOURCE: Science of Synthesis (2005), 18, 65-320

CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

ABSTRACT:

A review of the application of carbon dioxide, carbonyl sulfide, carbon disulfide, isocyanates, isothiocyanates, carbodiimides, and their selenium, tellurium, and phosphorus analog to organic synthesis.

=> DIS L11 2 IBIB IABS

L11 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:640828 CAPLUS

DOCUMENT NUMBER: 131:272178

TITLE: Preparation of N-(mercaptoalkyl)urea derivatives of amino acids as inhibitors of TNF- $\alpha$  production

INVENTOR(S): Mita, Shiro; Horiuchi, Masato; Ban, Masakazu; Suhara, Hiroshi

PATENT ASSIGNEE(S): Santen Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 324 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

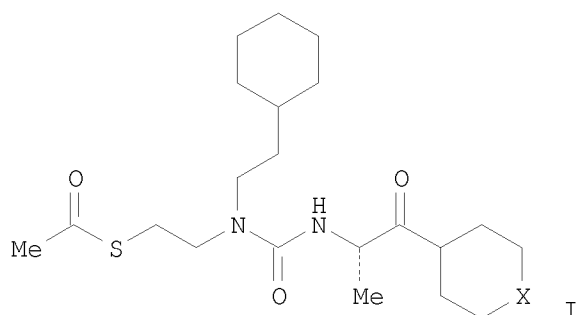
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.   | KIND | DATE     | APPLICATION NO. | DATE     |
|--|------|----------|-----------------|----------|
| -----  | ---- | -----    | -----           | -----    |
| WO 9950238   | A1   | 19991007 | WO 1999-JP1554  | 19990325 |
| W: CA, CN, KR, NO, US  |      |          |                 |          |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE |      |          |                 |          |

|   |    |          |                   |             |
|---|----|----------|-------------------|-------------|
| JP 2000044533   | A  | 20000215 | JP 1999-78346     | 19990323    |
| JP 3603177  | B2 | 20041222 |                   |             |
| CA 2325741  | A1 | 19991007 | CA 1999-2325741   | 19990325    |
| CA 2325741  | C  | 20070508 |                   |             |
| EP 1072591  | A1 | 20010131 | EP 1999-910724    | 19990325    |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI |    |          |                   |             |
| US 6492370  | B1 | 20021210 | US 2000-623779    | 20000908    |
| US 20020198376  | A1 | 20021226 | US 2002-147131    | 20020515    |
| US 6730784  | B2 | 20040504 |                   |             |
| PRIORITY APPLN. INFO.:  |    |          | JP 1998-79154     | A 19980326  |
|   |    |          | WO 1999-JP1554    | W 19990325  |
|   |    |          | US 2000-623779    | A3 20000908 |
| OTHER SOURCE(S):  |    |          | MARPAT 131:272178 |             |
| GRAPHIC IMAGE:  |    |          |                   |             |



#### ABSTRACT:

Prepared are  $\alpha$ -[N'-(mercaptoalkyl)ureido]alkanamide compds. having a urea structure as the basic structure and carrying sulfur and amide bonds in side chains. The above compds. are represented by general formula R1S-A1(R7)-NR2CONR3-A2(R4)CONR5R6 [wherein R1 represents H, (un)substituted lower alkyl or aromatic group, RA-CO-, RC-S- or a group of formula S-A1(R7)-NR2CONR3-A2(R4)CONR5R6; R2, R3 and R4 represent each H, (un)substituted lower alkyl or alkenyl, cycloalkyl, cycloalkenyl or (un)substituted aromatic group; R5 and R6 represent each H, (un)substituted lower alkyl or alkenyl, cycloalkyl, cycloalkenyl or (un)substituted aromatic group, or R5 and R6 may form together (un)substituted nonarom. heterocycle; R7 represents H, (un)substituted lower alkyl, cycloalkyl, hydroxy, mercapto, Ph, RB-O-, RC-S-, RD-COS-, RE-OCO-, RF-N(RG)- or -CONHOH; A1 and A2 represent each an alkylene; RA represents lower (halo)alkyl, aromatic group, lower alkoxy, aromatic-lower alkoxy, RF, or NRG; RB represents lower alkyl or aromatic group; RC represents H, lower alkyl, aromatic group; RD represents lower alkyl or aromatic group; RE represents H, lower alkyl, or aromatic group, RF and RG represent H, lower alkyl, cycloalkyl, or aromatic group]. It has been found out that these compds. have pharmacol. effects, in particular, a tumor necrosis factor- $\alpha$  (TNF- $\alpha$ ) production inhibitory effect. They are useful as remedies for autoimmune diseases and as antirheumatics. Thus, (2S)-2-[3-[2-(acetylthio)ethyl]-3-(2-cyclohexylethyl)ureido]propionic acid (preparation given) was condensed with N-methylpiperazine using 1-hydroxybenzotriazole, 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride, and N-methylmorpholine in CH<sub>2</sub>Cl<sub>2</sub> at room temperature overnight to give the title compound (I; X = NMe) in 78% yield. I (X = NMe) and I (X = O) at 50 mg/kg p.o. inhibited the Salmonella lipopolysaccharide-induced production of TNF- $\alpha$  in rats by 84.6 and 93.5%, resp.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> DIS L11 3 IBIB IABS

L11 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:637443 CAPLUS

DOCUMENT NUMBER: 125:329473

TITLE: Preparation of aminediol-containing peptide analogs as retroviral protease inhibitors

INVENTOR(S): Gordon, Eric M.; Barrish, Joel C.; Bisacchi, Gregory S.; Sun, Chong-qing; Tino, Joseph A.; Vite, Gregory D.; Zahler, Robert

PATENT ASSIGNEE(S): E. R. Squibb & Sons, Inc., USA

SOURCE: U.S., 219 pp., Cont.-in-part of U.S. Ser. No. 927,027, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

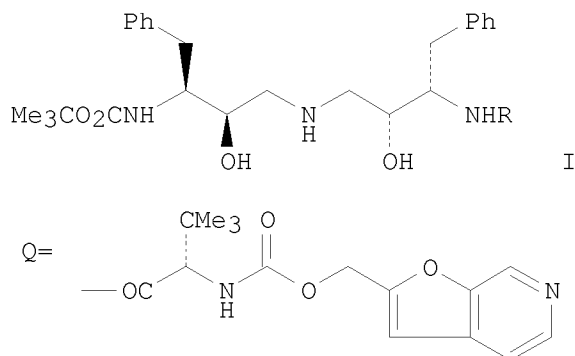
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE        |
|---|------|----------|-----------------|-------------|
| US 5559256  | A    | 19960924 | US 1993-79978   | 19930625    |
| AU 9341659  | A    | 19940127 | AU 1993-41659   | 19930630    |
| AU 677194   | B2   | 19970417 |                 |             |
| HU 67090  | A2   | 19950130 | HU 1993-2080    | 19930719    |
| CA 2100894  | A1   | 19940121 | CA 1993-2100894 | 19930720    |
| NO 9302620  | A    | 19940121 | NO 1993-2620    | 19930720    |
| EP 580402   | A2   | 19940126 | EP 1993-305691  | 19930720    |
| EP 580402   | A3   | 19970305 |                 |             |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE |      |          |                 |             |
| ZA 9305243  | A    | 19940217 | ZA 1993-5243    | 19930720    |
| CN 1085546  | A    | 19940420 | CN 1993-108954  | 19930720    |
| JP 06206857   | A    | 19940726 | JP 1993-201016  | 19930720    |
| US 5760036  | A    | 19980602 | US 1995-455295  | 19950531    |
| US 5776933  | A    | 19980707 | US 1995-456125  | 19950531    |
| PRIORITY APPLN. INFO.:  |      |          | US 1992-916916  | B2 19920720 |
|   |      |          | US 1992-927027  | B2 19920806 |
|   |      |          | US 1993-79978   | A 19930625  |

OTHER SOURCE(S): MARPAT 125:329473

GRAPHIC IMAGE:



## ABSTRACT:

Aa-E-NR8CHR9H(OH)CH2NHCH2CH(OH)CHR9NR8-E-Ab [Aa, Ab = H, alkyl, R3C(:Z), R3SO2, R3R4NSO2, R3R4NC(:Z), R3SC(:O), R5R6R7COC(:Z); E = a single bond or a peptide chain containing 1 to 4 amino acids, the N-terminus of which is bonded to Aa or Ab; R3, R4 = H, alkyl, aryl, carbocyclyl; R5, R6, R7 = H, alkyl, aryl, carbocyclyl, fluorenyl, alkynyl, alkenyl; R5, R6, and R7 may, independently, be joined together with the carbon atom to which they are bonded, to form a mono-, bi- or tricyclic carbocyclic ring system; R8 = H, alkyl; R9 = arylalkyl; Z = O, S; wherein: wherever they appear alone or as part of another group, unless otherwise indicated, the terms "alkaline" or "alkyl" denote a straight or branched chain saturated radical containing 1 to 12 carbons in the normal chain, optionally substituted by one or more groups selected from (un)protected OH, oxo (with the proviso that the carbon bearing the oxo group is not adjacent to a heteroatom), CO2H, halo, alkoxy, aryloxy, alkoxy carbonyl, etc.] or salts thereof, which inhibit retroviral protease and are particularly useful in the treatment and/or prevention of HIV infection (AIDS), are prepared Thus, bis(3-amino-2-hydroxy-4-phenylbutyl)amine derivative (I; R = H) was condensed with L-tert-leucine derivative (HO-Q) using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and HOBt in DMF/CH2CH2 at 0° to room temperature to give the title compound I (R = Q). The latter compound at 10 µM in vitro inhibited 99% HIV protease and showed IC50 of 0.012 µM which was the concentration of drug that increased the formazan production in CEM-SS cells infected with the RF strain of HIV to 50% of that produced by uninfected cells in the absence of drug.

=&gt; DIS L11 4 IBIB IABS

L11 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:379301 CAPLUS  
DOCUMENT NUMBER: 125:59147  
TITLE: Preparation of stable analogs of bioactive peptides  
containing disulfide linkages  
INVENTOR(S): Srinivasan, Ananthachari; Lyle, Leon R.; Rajagopalan,  
Raghavan  
PATENT ASSIGNEE(S): Mallinckrodt Medical, Inc., USA  
SOURCE: PCT Int. Appl., 35 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

| PATENT NO.   | KIND             | DATE     | APPLICATION NO. | DATE        |
|--|------------------|----------|-----------------|-------------|
| -----  | ---              | -----    | -----           | -----       |
| WO 9603429   | A1               | 19960208 | WO 1995-US9041  | 19950718    |
| W: CA, HU, JP  |                  |          |                 |             |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE |                  |          |                 |             |
| US 6664367   | B1               | 20031216 | US 1994-278437  | 19940721    |
| CA 2195525   | A1               | 19960208 | CA 1995-2195525 | 19950718    |
| EP 776334  | A1               | 19970604 | EP 1995-926734  | 19950718    |
| R: AT, DE, ES, FR, GB, IT, NL                                      |                  |          |                 |             |
| JP 10503205  | T                | 19980324 | JP 1996-505827  | 19950718    |
| EP 1132394   | A1               | 20010912 | EP 2001-201487  | 19950718    |
| R: AT, DE, ES, FR, GB, IT, NL                                      |                  |          |                 |             |
| PRIORITY APPLN. INFO.:   |                  |          | US 1994-278437  | A 19940721  |
|  |                  |          | EP 1995-926734  | A3 19950718 |
|  |                  |          | WO 1995-US9041  | W 19950718  |
| OTHER SOURCE(S):   | MARPAT 125:59147 |          |                 |             |
| GRAPHIC IMAGE:   |                  |          |                 |             |



INVENTOR(S): Evans, Christopher J.; Valentino, Karen L.; Bassett, Patricia M.; Singh, Tejinder; Yamashiro, Donald H.  
 PATENT ASSIGNEE(S): Neurex Corp., USA  
 SOURCE: PCT Int. Appl., 35 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.   | KIND | DATE     | APPLICATION NO. | DATE       |
|--|------|----------|-----------------|------------|
| WO 9204633   | A1   | 19920319 | WO 1991-US6115  | 19910827   |
| W: AU, CA, FI, JP, KR                                  |      |          |                 |            |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE |      |          |                 |            |
| AU 9184996   | A    | 19920330 | AU 1991-84996   | 19910827   |
| PRIORITY APPLN. INFO.:                                 |      |          | US 1990-577870  | A 19900905 |
|  |      |          | WO 1991-US6115  | A 19910827 |

OTHER SOURCE(S): MARPAT 117:44064

ABSTRACT:

A method and antibody (Ab) composition are disclosed for screening biol. material for the presence of bioactive peptides. The Ab composition includes >1 Abs immunoreactive with (1) different amidated carboxyl-terminal amino acid residues, (2) different amino-terminal Pyroglu amino acid residues, or (3) a combination of group 1 and 2 antigens. In the method, the Ab composition is reacted with the material to be screened, and the material is then examined for the presence of immunoconjugate. Thus, anti-valinamide antisera were prepared (using a valinamide-thyroglobulin conjugate for immunogen). The antisera labeled areas of the brain and pituitary in a pattern consistent with the distribution of 2 known carboxyl-terminal valinamide peptides, metorphamide, and  $\alpha$ -MSH. Immunoassays for other bioactive peptides are also described, as is preparation of a branched linker conjugate immunogen.

=> DIS L11 6 IBIB IABS

L11 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:439848 CAPLUS

DOCUMENT NUMBER: 111:39848

ORIGINAL REFERENCE NO.: 111:6801a,6804a

TITLE: Synthesis of peptides containing S-(N-alkylcarbamoyl)cysteine residues, metabolites of N-alkylformamides in rodents and in humans

AUTHOR(S): Threadgill, Michael D.; Gledhill, Adrian P.

CORPORATE SOURCE: Pharm. Sci. Inst., Aston Univ., Birmingham, B4 7ET, UK

SOURCE: Journal of Organic Chemistry (1989), 54(12), 2940-9

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:39848

ABSTRACT:

Hydrochloride salts of S-(N-methylcarbamoyl), S-(N-ethylcarbamoyl), and S-(N,N-dimethylcarbamoyl) derivs. of cysteine, N-acetylcysteine, and cysteinylglycine have been prepared S-(N-Methylcarbamoyl)glutathione hydrochloride has also been synthesized. Protecting groups for amino and carboxylic acid functions were selected for their ability to solubilize the peptides in CH<sub>2</sub>Cl<sub>2</sub>, the solvent in which the thiols were treated with alkyl isocyanates and with Me<sub>2</sub>NCOC<sub>2</sub>H<sub>5</sub>. Removal of S-(amidomethyl) protecting groups using Hg(OAc)<sub>2</sub> caused some loss of N-(tert-butoxycarbonyl) groups. Elimination of disulfide was evident during coupling of disulfide derivs. of cysteine using mixed anhydride methods but not with a carbodiimide coupling agent.

Mixed disulfide protections were reductively cleaved by HS(CH<sub>2</sub>)<sub>3</sub>SH. Many of the deprotected S-carbamoyl amino acids and peptides are metabolites of the corresponding N-alkylformamides in rodents and in humans.

=> DIS L11 7 IBIB IABS

L11 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1953:6204 CAPLUS

DOCUMENT NUMBER: 47:6204

ORIGINAL REFERENCE NO.: 47:1054b-g

TITLE: Peptides. II. Selective degradation by removal of the terminal amino acid bearing a free amino group. The use of alkyl alkoxydithioformates (dialkyl xanthates)

AUTHOR(S): Kenner, G. W.; Khorana, H. G.

CORPORATE SOURCE: Univ. Cambridge, UK

SOURCE: Journal of the Chemical Society (1952) 2076-81

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 47:6204

ABSTRACT:

Peptides are converted by the action of MeSC(:S)OR on their salts in H<sub>2</sub>O at room temperature into their N-thionocarbalkoxy derivs. These substances are cleaved by HCl in MeNO<sub>2</sub> to the HCl salt of an amino acid or degraded peptide and a 4-alkyl-2,5-thiazolidinedione, from which the terminal amino acid may be regenerated by mild hydrolysis. The two steps proceed in almost quant. yield and in combination constitute a valuable method for selective degradation of peptides. O-Bu Me xanthate, light yellow, b<sub>0.5</sub> 60°.

MeCH(NH<sub>2</sub>)CONHCH<sub>2</sub>CO<sub>2</sub>H (0.146 g.) in 0.22 cc. 5 N NaOH, treated with 0.52 g. EtOC(:S)SMe and then with about 1 cc. EtOCH<sub>2</sub>CH<sub>2</sub>OH, kept 48 hrs. at 18-20°, evaporated in vacuo, diluted with 5 cc. H<sub>2</sub>O, extracted 3 times with ether, and the aqueous solution treated with 1 cc. AcOH, extracted with AcOEt, and the acidification and extraction repeated, gives 86% N-thionocarbethoxy-D-alanylglycine (I), m. 143-4°; the DL-valine analog m. 98° and the DL-proline analog m. 128-9°. I in anhydrous MeNO<sub>2</sub>, saturated with dry HCl (complete exclusion of moisture), gives 70% of H<sub>2</sub>NCH<sub>2</sub>CO<sub>2</sub>H.HCl (II); the residue from the MeNO<sub>2</sub> solution, treated with N NaOH, and acidified with HCl, gives DL-MeCH(NH<sub>2</sub>)CO<sub>2</sub>H; it is believed that the latter is present initially as the 2,5-thiazolidinedione which is too unstable for isolation. The degraded dipeptide can be extracted from the MeNO<sub>2</sub> with H<sub>2</sub>O, transformed into the Na salt, and treated with another portion of ROC(:S)SMe. The following

N-thionocarbethoxy compds. were prepared and degraded by the above method:

DL-leucylglycine, m. 122°, quant. yield (II and DL-leucine);

glycylglycine, m. 142-3° (degradation not entirely satisfactory since warm MeNO<sub>2</sub> needed); glycyl-DL-valine, m. 131-2°, quant. yield (DL-valine isolated in 0.5 hr.); glycyl-DL-leucine, m. 109-10°, 84% (one sample m. partly at 110° and completely at 120°) (DL-leucine);

glycy-DL-phenylalanine, m. 74-5°, quant. yield, DL-Leucylglycylglycine, m. 126-7°, 93% (glycylglycine-HCl formed). N-

(Thionocarbobutoxy)glycylglycine, m. 84-5° (degradation yields II); the glycylglycylglycine m. 152-3°, 82%. DL-Alanylglycine and Na

1,2,4-naphthaquinonesulfonate give (24 hrs.) a red solution; acidification and extraction with BuOH give a red compound, the aqueous solution of which is decolorized by

Ague or H<sub>2</sub>O<sub>2</sub>; traces of H<sub>2</sub>NCH<sub>2</sub>CO<sub>2</sub>H were isolated. No appreciable reaction was noted between MeCH(NH<sub>2</sub>)CO<sub>2</sub>H or MeCPh(NH<sub>2</sub>)CO<sub>2</sub>H and HCS<sub>2</sub> Na in 48 hrs.

DL-Alanylglycine and CH<sub>2</sub>:CHCN in N NaOH, shaken 24 hrs., give 72%

N-2-cyanoethyl-DL-alanylglycine, m. 150°; N alkali at room temperature or MeONa in boiling PhMe give some H<sub>2</sub>NCH<sub>2</sub>CO<sub>2</sub>H.

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COST IN U.S. DOLLARS

| SINCE FILE | TOTAL   |
|------------|---------|
| ENTRY      | SESSION |
| 26.53      | 425.28  |

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|------------|---------|
| ENTRY      | SESSION |
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PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
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FULL ESTIMATED COST

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| SINCE FILE | TOTAL   |
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| ENTRY      | SESSION |
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L1 STRUCTURE UPLOADED

L2 50 S L1 SSS SAM

L3 9686 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 06:41:58 ON 20 MAY 2008

L4 5006 S L3

L5 12 S L4 AND THIOCARBAMIDE

FILE 'REGISTRY' ENTERED AT 07:09:00 ON 20 MAY 2008

L6 SCREEN 1994

L7 STRUCTURE UPLOADED

L8 QUE L7 AND L6

L9 50 S L8 SSS SAM

L10 3337 S L8 SSS FULL

FILE 'CAPLUS' ENTERED AT 07:09:43 ON 20 MAY 2008

E CARBODIIMIDE+ALL/CT

L11 7 S L10 AND (CARBODIIMIDE OR "CARBODIIMIDES")

=> file caplus

|  |            |         |
|--|------------|---------|
| COST IN U.S. DOLLARS                       | SINCE FILE | TOTAL   |
| FULL ESTIMATED COST                        | ENTRY      | SESSION |
|  | 27.01      | 425.76  |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL   |
| CA SUBSCRIBER PRICE                        | ENTRY      | SESSION |
|  | -5.60      | -15.20  |

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FILE 'REGISTRY' ENTERED AT 06:40:38 ON 20 MAY 2008

L1 STRUCTURE UPLOADED  
 L2 50 S L1 SSS SAM  
 L3 9686 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 06:41:58 ON 20 MAY 2008

L4 5006 S L3  
 L5 12 S L4 AND THIOCARBAMIDE

FILE 'REGISTRY' ENTERED AT 07:09:00 ON 20 MAY 2008

L6 SCREEN 1994  
 L7 STRUCTURE UPLOADED  
 L8 QUE L7 AND L6  
 L9 50 S L8 SSS SAM  
 L10 3337 S L8 SSS FULL

FILE 'CAPLUS' ENTERED AT 07:09:43 ON 20 MAY 2008

E CARBODIIMIDE+ALL/CT  
 L11 7 S L10 AND (CARBODIIMIDE OR "CARBODIIMIDES")

FILE 'CAPLUS' ENTERED AT 07:24:32 ON 20 MAY 2008

=> s l4 and "thiocarbamic ester"  
 606 "THIOCARBAMIC"  
 620555 "ESTER"  
 12 "THIOCARBAMIC ESTER"

L12 ("THIOCARBAMIC"(W)"ESTER")  
1 L4 AND "THIOCARBAMIC ESTER"

=> DIS L12 1 IBIB IABS

L12 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:949272 CAPLUS

DOCUMENT NUMBER: 124:7965

ORIGINAL REFERENCE NO.: 124:1689a,1692a

TITLE: Reductive cleavage of dithiocarbamic esters and  
thiocarbamic esters promoted by samarium(II) diiodide

AUTHOR(S): Jiang, Hua-Jiang; Zhang, Yong-Min

CORPORATE SOURCE: Department of Chemistry, Hangzhou University,  
Zhijiang, 310028, Peop. Rep. China

SOURCE: Youji Huaxue (1995), 15(5), 481-6

CODEN: YCHHDX; ISSN: 0253-2786

PUBLISHER: Kexue

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

OTHER SOURCE(S): CASREACT 124:7965

ABSTRACT:

The reductive cleavage of dithiocarbamic esters are promoted by the  
SmI<sub>2</sub>-HMPA-THF-tert-BuOH system successfully to give disulfides and  
thiocarboxamides at room temperature in good yields; the reduction of thiocarbamic  
esters

are also promoted by the same system to give disulfides and carboxamides.

=> s l10 and "thiocarbamic ester"

1759 L10

606 "THIOCARBAMIC"

620555 "ESTER"

12 "THIOCARBAMIC ESTER"

("THIOCARBAMIC"(W)"ESTER")

L13 0 L10 AND "THIOCARBAMIC ESTER"

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COST IN U.S. DOLLARS

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TOTAL

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FULL ESTIMATED COST

12.83

438.59

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